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This paper examines the problem of "positivity" in relation to the partial realization of scalar power series. An exact criterion of positivity is proved for second-order realizations. The general case is currently unsolved. Even the special results contained here show that the so-called "maximum entropy principle" cannot be applied to the realization problem in the naive sense in which it is employed by physicists. It would be better to call this principle a "prejudice" because it does not fully utilize the information inherent in the data and does not provide a realization with natural ("minimal") mathematical properties.

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REALIZATION OF COVARIANCE SEQUENCES*

R. E. Kalman

This paper examines the problem of "positivity" in relation to the partial realization of scalar power series. An exact criterion of positivity is proved for second-order realizations. The general case is currently unsolved. Even the special results contained here show that the so-called "maximum entropy principle" cannot be applied to the realization problem in the naive sense in which it is employed by physicists. It would be better to call this principle a "prejudice" because it does not fully utilize the information inherent in the data and does not provide a realization with natural ("minimal") mathematical properties.

The research I planned to report on is unfortunately not yet completed. So the following is only an outline of the problem. It has been around for a long time without receiving a definitive solution. It occupies quite a central position in system theory and has been frequently misinterpreted. It is not in the least controversial but it is unsolved.

As perhaps the only algebraist at this meeting, it is safer for me if I use a reasonably nontechnical language. In such terms, the topic of my paper is: What is the relation between partial realizations and positivity?

Evidently I must now define "partial realization" and (in relation to it) "positivity".

To take the simplest (scalar) case, consider an arbitrary sequence of numbers from a fixed field k ,

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$$(1) \quad a_1, a_2, \dots, a_t, \dots$$

This sequence may be interpreted as an element

$$(2) \quad \sigma(z^{-1}) = \sum_{s>0} a_s z^{-s}$$

of the ring of formal power series $z^{-1}k[[z^{-1}]]$. (We shall always adhere to the normalization convention that $a_0 = 0$.)

Consider now any (irreducible) rational fraction written formally as $\pi_t(z)/\chi_t(z)$, with coefficients in k , with χ_t monic, and with $\deg \pi_t < \deg \chi_t$. Attached to each such fraction there is a (unique) formal power series which we write as

$$(3) \quad \pi_t(z)/\chi_t(z) = \sum_{s>0} b_s z^{-s}.$$

(Another normalization convention is that polynomials are written with indeterminate z while the corresponding power series are written with indeterminate z^{-1} .)

Let t be fixed or variable. We say that (π_t, χ_t) is a partial realization of (1) of order t iff

$$(4) \quad a_s = b_s, \quad s = 1, \dots, t.$$

There is a rather complete theory of partial realizations without any conditions on the sequence (1). An elementary account of this theory, sufficient for the present purposes, is in KALMAN [1979]. (A complete mathematical treatment will appear as KALMAN [1983].)

Assume that the field k is specialized to the reals \mathbb{R} . Assume also that the sequence (1) is replaced (change of notation to avoid conceptual confusion) by the sequence

$$(5) \quad c_0, c_1, c_2, \dots, c_t, \dots$$

or, equivalently,

$$(6) \quad c = \sum_{s=0}^{\infty} c_s z^{-s}.$$

To emphasize the conceptual difference between (1) and (5) we shall normalize the latter by setting $c_0 = 1$ (contrary to $a_0 = 0$).

We want to regard (5) as defined via the covariance function of a stationary random sequence $\{y_\tau\}$ with zero mean. That is,

$$(7) \quad E(y_\tau y_{\tau+s}) =: \text{cov}(y_\tau y_{\tau+s}) =: c_s = c_{-s}, \\ s = 0, \pm 1, \pm 2, \dots$$

(By stationarity, the left-hand side of (6) is independent of τ .) Each sequence (5) defines a sequence of Toeplitz matrices

$$(8) \quad T_t := \begin{bmatrix} 1 & c_1 & \dots & c_t \\ c_1 & 1 & \dots & c_{t-1} \\ \vdots & \ddots & & \vdots \\ \vdots & \ddots & & \vdots \\ c_t & c_{t-1} & \dots & 1 \end{bmatrix}.$$

Directly from the defining properties of "covariance", we see that (5) is a "covariance sequence", that is, defined by (7), if and only if each member of the infinite sequence

T_0, \dots, T_t, \dots is positive definite. This is the "positivity" property of the sequence (5) which we wish to study and which justifies the normalization $c_0 = 1$.

In other words, our basic problem will be: What happens to the theory of partial realizations if the sequence (5) is subjected to the additional condition $T_t > 0$?

In general, questions of "positivity" constitute an underdeveloped area of mathematics. Positivity is extremely important for system theory because it is directly related to questions of stochastic realization. The "identifiability" of noise and of stochastic effects comes about through the mathematical implications of positivity. (For some preliminary results along these lines, see KALMAN [1982].) Thus each theorem about positivity gives rise to a system-theoretic result. But more frequently, a system-theoretic question poses an (open) mathematical problem.

The classical results concerning "positivity" in relation to the sequence (5) were first elucidated in the study of orthogonal polynomials. Our favorite recent reference for this material is GERONIMUS [1961].

As in the theory of orthogonal polynomials, it is useful for us to introduce the sequence

$$(9) \quad r = (r_1, r_2, \dots, r_t, \dots),$$

sometimes called SCHUR parameters, defined from (5) by

$$(10) \quad r_t := (-1)^{t-1} (\det T_{t-1})^{-1} \det \begin{bmatrix} c_1 & c_2 & \dots & c_{t-1} & c_t \\ 1 & c_1 & \dots & c_{t-2} & c_{t-1} \\ \vdots & \vdots & & \vdots & \vdots \\ c_{t-2} & c_{t-3} & \dots & 1 & c_1 \end{bmatrix}.$$

For any positive infinite sequence (5), the infinite sequence r is well defined. The classical result is that (5) is a positive sequence if and only if $|r_t| < 1$ for all $t = 1, 2, \dots$.

By elementary arguments based on (8) and (10) it can be shown that there is a bijective correspondence, for each $t > 0$, between positive partial sequences

$$\{1, c_1, \dots, c_t\} \longleftrightarrow \{r_1, \dots, r_t\}.$$

Any partial realization problem may be viewed as looking for an infinite continuation of a finite sequence. By the bijection between c and r , the solution of the positive partial realization problem is then equivalent to finding a continuation of (9) by r_{t+1}, r_{t+2}, \dots so that $|r_{t+u}| < 1$ for all $u = 1, 2, \dots$. It is not clear, however, what continuations of r correspond (via the bijection) to rational continuations of c as required in the definition of the partial realization problem.

There is just one well-known fact concerning such continuations. The special continuation given by $r_s = 0$ for all $s = t + 1, t + 2, \dots$ is a rational

positive continuation of l, c_1, \dots, c_t and corresponds to a solution of the partial realization problem with $\deg x_t = t$.

This would seem to provide a solution to our problem. In fact, although the trick described above is mathematically quite trivial, the realization corresponding to $r_s = 0$, $s > t$, has been glorified by physicists by naming it the MAXIMUM ENTROPY PRINCIPLE. (See LEVINE and TRIBUS [1978] for recent speculations and references.) The terminology is due to the fact that continuation of (5) with $r_s = 0$ maximizes the classical (SHANNON) value of entropy. See (17-18) and below.

In mathematical terms, big talk like "maximum entropy" PRINCIPLE would seem to imply that the solution of the partial realization problem afforded by the above trick has some "natural" attributes. Unfortunately, this is far from true. There is a misunderstanding on the part of the physicists. SHANNON entropy does not represent the correct "information" measure for the realization problem discussed here. (Of course, SHANNON never claimed such a thing. The confusion arises from identifying "entropy" as technically defined by SHANNON with the word "information" and then wildly extrapolating the intuitive meaning of the latter.)

That the conventional application of the "maximum entropy" idea is incorrect in this context is easily seen from the fact that the preceding solution of the positive partial realization problem is not minimal, in the sense that $n_t := \deg x_t$ is not necessarily minimal among the family of all (rational) continuations of the sequence l, c_1, \dots, c_t . Nonminimal realizations are objectionable from the system-theoretic viewpoint as they do not provide the "simplest" explanation of the given data l, c_1, \dots, c_t .

To make these statements more precise, we now define the polynomials

$$(11a) \quad \phi_t(z) := (\det T_{t-1})^{-1} \det \begin{bmatrix} 1 & c_1 & \dots & c_t \\ c_1 & 1 & \dots & c_{t-1} \\ \vdots & \vdots & & \vdots \\ 1 & z & \dots & z^t \end{bmatrix} \quad (\phi_0(z) = 1),$$

and

$$(11b) \quad \phi_t^*(z) := z^{\deg \phi_t} \cdot \phi_t(z^{-1}).$$

These polynomials arise naturally in the well-known recursion relations in the theory of orthogonal polynomials, namely

$$(12a) \quad \phi_{t+1}(z) = z\phi_t(z) - r_{t+1}\phi_t^*(z),$$

$$(12b) \quad \phi_{t+1}^*(z) = -r_{t+1}\phi_t(z) + \phi_t^*(z).$$

Next, we need a little algebra. Let

$$(13) \quad (c, \pi) \mapsto \langle c, \pi \rangle := (c\pi)_{0\text{-th coefficient}}$$

be an abstract inner product between power series and polynomials; the product $c\pi$ is to be taken in the usual sense. Inserting (13) into the determinant defining ϕ_t gives $\langle c, \phi_t \rangle \equiv 0$ for all t . More generally,

$$(14) \quad r_t = \frac{\langle c, z\phi_{t-1} \rangle}{\langle c, \phi_{t-1}^* \rangle} = -\phi_t(0);$$

this follows immediately by applying the identity $\langle c, \phi_t \rangle \equiv 0$ to (12a). Formula (14) is mildly original.

Now it is easy to see what the condition $r_s = 0$, $s > t$, amounts to.

By formula (14), we get

$$(15) \quad \langle c, z\phi_s \rangle = 0 \quad \text{for } s \geq t.$$

By induction, this implies

$$(16) \quad \langle c, z^u \phi_t \rangle = 0 \quad \text{for } u = 1, 2, \dots .$$

Using also (11a), relations (16) express the fact that ϕ_t is a recursion polynomial for the sequence $1, c_1, \dots, c_t$ extended to an infinite sequence by the assumption $r_s = 0$, $s > t$. Defining $x_t := \phi_t$ gives a solution of the positive partial realization problem.

Note that ϕ_t is a recursion polynomial for the finite sequence $c_{t-1}, c_{t-2}, \dots, c_0, c_1, \dots, c_t$ for each t .

The entropy associated with a covariance of length t is defined in the sense of SHANNON as

$$(17) \quad H_t := \frac{1}{2} \log \det T_t.$$

Note that $\det T_t / \det T_{t-1} = \langle c, \phi_t^* \rangle$ by (11a). Then, using (12b), we get immediately

$$(18) \quad \frac{\det T_{t+1}}{\det T_t} = (1 - r_{t+1}^2) \frac{\det T_t}{\det T_{t-1}}.$$

This shows that $r_s = 0$ for $s > t$ is indeed that continuation of r_1, \dots, r_t which maximizes SHANNON's entropy

$$H_{t+1}, H_{t+2}, \dots .$$

Let us investigate the simplest special cases of this result.

Case $t = 1$. Here the application of partial realization theory is trivial: all minimal partial realizations of the sequence $1, c_1$ are given by the fraction $z/(z - c_1)$. From formula (11a) we see that $x_1(z) = (z - c_1)$ is identical with $\phi_1(z)$ of the maximum entropy realization. (This is just a lucky coincidence.) The positivity condition on the minimal partial realization is $|r_1| = |c_1| < 1$. Since the parameter c_1 is "free" in the minimal partial realization problem, here the positivity requirement does not interfere with the minimality requirement. (In the fraction for the partial realization the factor z is due to the different normalization of (5) vs. (1).)

It would be a great mistake, however, to imagine that this is typical of the general situation.

Case $t = 3$. Here we study positive minimal partial realizations of the partial sequence $1, c_1, c_2, c_3$. If $c_2 \neq c_1^2$ then the minimal realization problem has a "jump" of size 1 at $t = 2$ (see KALMAN [1979]), c_3 is a free parameter, and $n_3^{\min} = 2$. (If $c_2 = c_1^2$ but $c_3 \neq c_1^3$ then the minimal partial realization problem has a jump of size 2 at $t = 3$, so that now c_4 and c_5 are free parameters, and $n_5^{\min} = 3$. This case is already rather difficult to analyze.)

We assume $c_2 \neq c_1^2$ which is equivalent to $r_2 \neq 0$. Then the minimal partial realization is given by the finite continued fraction

$$(19) \quad \frac{z}{z - r_1 - \frac{r_2(1 - r_1^2)}{z + r_1 r_2 - \frac{r_3(1 - r_2^2)}{r_2}}} .$$

The conditions

$$(20) \quad |r_1| < 1, \quad |r_2| < 1, \quad |r_3| < 1$$

are obviously necessary for the partial sequence $1, c_1, c_2, c_3$ to be positive, irrespective of the assumed jump pattern. These positivity conditions can be easily satisfied without conflicting with the minimality requirements of the partial realization; r_1 and r_3 are free parameters and the condition $r_2 \neq 0$ does not interact with $|r_2| < 1$.

But (20) is not sufficient to insure that the infinite sequence generated by (19) is positive! The necessary and sufficient condition for the latter requirement is (after rather extensive calculations) found to be

$$(21) \quad |r_3| < \frac{|r_2|}{1 + |r_2|} < \frac{1}{2} .$$

This is much stronger than $|r_3| < 1$. Thus, the positivity conditions on a partial sequence are not sufficient to guarantee that the corresponding minimal partial realizations generate a positive (infinite) sequence.

When r_3 does not satisfy (21), the minimal partial realization of $1, c_1, c_2, c_3$ (assuming $c_2 \neq c_1^2$) is not positive; conversely, the minimal positive partial realization of this sequence is then at least of degree 3 (but not higher, because of the existence of the maximum entropy realization).

The preceding investigation, which is of course mathematically rigorous, shows that for $t = 3$ the maximum entropy realization is not necessarily a "natural" realization since there may exist a minimal realization of degree 2. (If $1, c_1, c_2, c_3$ corresponds to $r_1, 0, 0$ then $\Phi_3(z) = z^2\Phi_1(z)$ so that the maximum entropy principle does provide the unique minimal realization of degree 1. But this is just another lucky accident.)

If it is true that the maximum entropy principle fails to reliably select the simplest (here "minimal") realization, then this alleged organizing principle of nature must contain some extraneous assumptions (which I propose to designate by the technical term prejudice, as in KALMAN [1982]). What are these extraneous assumptions? Where does the prejudice come in?

JAYNES [1968] describes the principle as follows:

"The [prior probability assignment] that describes the available information but is maximally noncommittal with regard to the unavailable information is the one with maximum entropy (my italics)."

It is hard to quarrel with this statement on intuitive grounds. Everything hinges on the meaning given to the word "information". JAYNES and his followers apparently blindly accept that SHANNON entropy = information. But entropy is never a measure of "available information" of the mathematical type.

In the literature (see, for example, ULRYCH and BISHOP [1975]) the maximum-entropy realization is regarded as equivalent to estimation by the autoregressive (AR) method. (This is in fact easily proved with the help of the machinery developed here.) Thus "maximum entropy" becomes a "higher" justification for the AR method or vice versa. But the AR method is also objectionable; it implies the tacit assumption (prejudice) that the partial realization problem consists of one concentrated jump---which is a highly nongeneric case.

The problem of attempting to apply the maximum entropy dictum of JAYNES via formulas (17-18) is simply that the SHANNON entropy does not correctly measure the "available information" provided by values of r_1, \dots, r_t . This is not a question of probabilities; the computation of $\Phi_t(z)$ is based on the exact knowledge of r_1, \dots, r_t .

Consider again (19). If $r_2 \neq 0$ but $|r_2|$ is small then by (20) $|r_3|$ must be small also and therefore $\chi_2(z)$, the denominator of (19) viewed as an ordinary fraction, is very close to $\Phi_1(z) = z - r_1$. This means that the correct (minimal) solution of the partial realization problem is very similar to the case where the only data is r_1 , even though r_2 and r_3 are not exactly zero.

On the other hand, if $|r_2|$ is nearly 1 then $\chi_2(z)$ will differ from $\Phi_2(z)$ only by a term bounded by $1 - |r_2|$ while $|r_3|$, far from being required to be zero as by the maximum entropy method, can be almost as large as 1/2.

We see that the realizations provided by the maximum entropy prejudice are approximately valid in a much wider range than the rigid assumption that $|r_s| = 0$ for $s > t$. To see whether $\Phi_{t_1}(z)$, $t_1 < t$ is approximately valid for the sequence $1, c_1, \dots, c_{t_1}, \dots, c_t$ we need certain bounds on $|r_{t_1+1}|$, $|r_{t_1+2}|, \dots$ which guarantee that the infinite continuation of the sequence by a partial realization of order t_1 is still

positive. It is these missing bounds which constitute the unsolved mathematical problem. Results of the writer at present are limited to (19) and its corresponding bound (21). In general, if $|r_s|$ is sufficiently small for $t_1 < s \leq t$, we may expect to get positive partial realizations that are much more efficient than the maximum entropy realization. Thus, to correctly implement JAYNES' intuitive principle, it is necessary to know the values of the $|r_s|$. On the other hand, the conventional application of the maximum entropy principle (designating $\Phi_t(z)$ as the recursion polynomial) uses the classical entropy formula (17) which requires only the "information" that $|r_s| < 1$ for $1 \leq s \leq t$; the actual values of r_s are used in constructing $\Phi_t(z)$ but not in applying (17).

Thus the prescription $r_s = 0$, $s > t$, should be regarded only as a realization of "last resort", precisely because in doing so we have not exploited all available information.

As soon as the mathematical problem posed here is solved, we would be in a position to implement JAYNES' desideratum of not throwing away any information concerning the sequence r_1, \dots, r_t . By working backward, we would then replace formula (17) by a different expression which would correctly measure "information" as it is relevant to the realization problem. Evidently the correct measure of "information" for a mathematical problem will not be the same as the measure of entropy for a physical problem.

"Entropy" is the measure of the lack of organization (structure) in a physical situation; it has nothing to do with the "system aspect" of things and therefore entropy is useless not only as a technical tool but also as a conceptual crutch. Were Nature so constituted that simple principles explain everything, "maximum entropy" would be one of the deep insights and we would not need Mathematics. But Nature, if sometimes simple, is often complicated and therefore Mathematics is indispensable.

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